Quantum Chemistry and Reaction Dynamics

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Quantum Chemistry and Reaction Dynamics

- **Ab initio Electronic Structure Theories, Methods, and Algorithms**
  - Dr. Robert J. Harrison, Oak Ridge National Laboratory
  - Dr. Martin Head-Gordon, Lawrence Berkeley National Laboratory
  - Professor Mark S. Gordon, Iowa State University and Ames Laboratory
  - Professor Piotr Piecuch, Michigan State University
  - Professor Peter R. Taylor, University of Warwick, UK
  - Professor Henry F. Schaefer III, University of Georgia
- **Electronic Structure Methods for Systems with Periodic Boundaries**
  - Professor Gustavo E. Scuseria, Rice University
- **Relativistic Quantum Chemistry**
  - Professor Russell M. Pitzer, The Ohio State University
  - Professor Walter C. Ermler, The University of Memphis
  - Professor Maria M. Marino, The University of Memphis
- **Thermochemistry, Kinetics, and Chemical Dynamics**
  - Dr. Albert F. Wagner, Argonne National Laboratory
  - Professor Donald L. Thompson, Oklahoma State University

Multiscale Approach to Combustion

"**Address the electronic structure, chemical kinetics, and fluid mechanics issues necessary to create a software revolution in the simulation of chemically reacting turbulent flows. To the degree that funding allows, the intention is to initiate a collaboration that will grow over time into a coordinated software development program.**"

Quantum Chemistry — Thermo-Chemistry — Kinetics — Mechanisms — Reaction Chemistry Simulations

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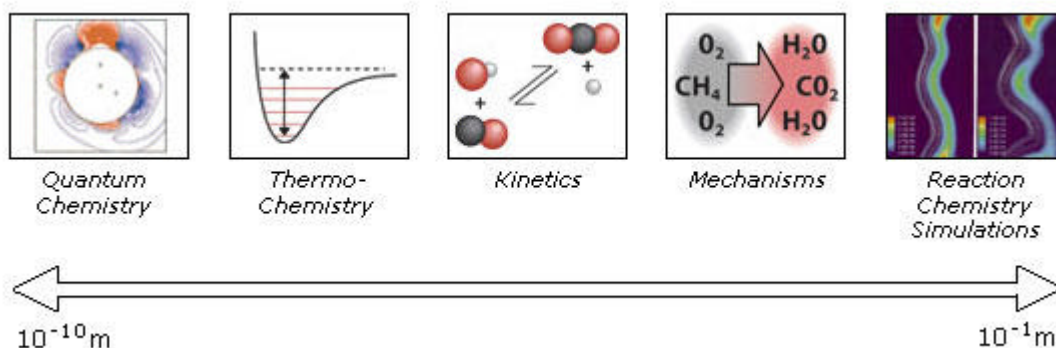
- Oak Ridge National Laboratory, *"Advanced Methods for Electronic Structure"*
- Argonne National Laboratory, *"Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamics"*
- Sandia National Laboratory, *"A Computational Facility for Reacting Flow Science"*
- *"Collaboratory for Multi-Scale Chemical Science"* – SNL, PNNL, ANL, LANL, LLNL, MIT, NIST, UCB, (Larry Rahn, PI)

Questions:

- How is the SciDAC team approach to science changing the way you conduct your research? [Research approach]

- What has your SciDAC project accomplished that has enabled scientists to better realize the potential of terascale computing? What science can be done now that was not previously possible? Please be specific about which application area(s) you have worked in and with whom. [Scientific accomplishments]

- What specific algorithmic or software tools or technology are you now able to provide to scientists to enable them to advance their research through the use of terascale computing? [New software capabilities]

- What are your plans for the next year or two in accomplishing SciDAC goals? Be as specific as possible about your interactions with other SciDAC teams. [Future plans]

- What computational resource needs do you anticipate, both high-end computing platforms and associated infrastructure (including networking), to accomplish your goals? [Computational resource needs]

A Guaranteed Precision and Speed – Multiresolution Quantum Chemistry

Robert J. Harrison and G.I. Fann, ORNL and Gregory Beylkin, University of Colorado

- Research approach
  - MRA, new separable representations for kernels of Green functions (in particular, Poisson and bound-state Helmholtz equations).
  - Prototype code written in Python, with C and Fortran for computationally intensive kernels; Python, a high-level, object-oriented scripting language, has greatly accelerated development.
  - Object-oriented design enables applications to be written at a very high level, composed in terms of operations performed upon functions.
  - Permits the application developer to focus upon the physics/chemistry instead of computational details.
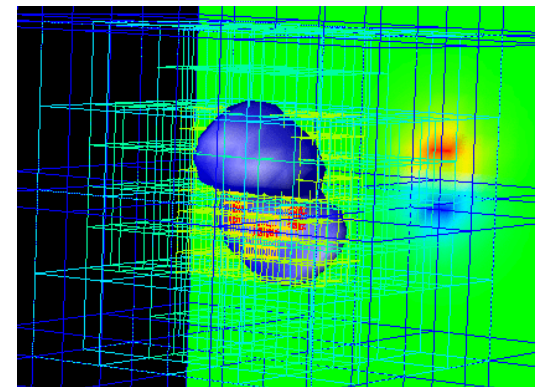
Molecular orbital of benzene showing the adaptively refined grid and an isosurface.

A Guaranteed Precision and Speed – Multiresolution Quantum Chemistry

Robert J. Harrison and G.I. Fann, ORNL and Gregory Beylkin, University of Colorado

- Scientific accomplishments
  - Effective one electron theories with the implementation and validation of a parallel, prototype computer code for density functional theory (DFT) and Hartree-Fock (HF) energies, analytic derivatives w.r.t. atomic positions, and linear response theory for excited states.
  - Code applied to atoms as heavy as barium and many molecules comprising first, second and third row atoms
- New software capabilities
  - Multiresolution adaptive numerical scientific simulation (MADNESS); includes classes that provide functions and operators in 1, 3 and 6 (limited capability to date) dimensions, with free-space boundary conditions and separated forms for critical kernels.

A Guaranteed Precision and Speed – Multiresolution Quantum Chemistry

Robert J. Harrison and G.I. Fann, ORNL and Gregory Beylkin, University of Colorado

- Future plans
    - Add other boundary conditions as operators as need arises.
    - Prototype other application areas within the same framework.
    - Next version of the code will use distributed memory and scale to many more processors.
    - More production-oriented computer program will draw more heavily upon the resources of the ISICs for scalable iterative solvers, visualization, CCA, and performance analysis.
    - Solution in six spatial dimensions.
- Computational resource needs
    - Access to massive computer resources in the Center for Computational Science at ORNL has enabled rapid exploration of the parameter space that control speed and precision.
    - The current parallel algorithm is limited to processors within a single shared memory computer, so the 32-processor IBM Power-4 nodes at ORNL have been particularly useful.

Accurate Properties for Open-Shell States of Large Molecules

Peter R. Taylor, University of Warwick

- Research approach
  - Efficient implementation profits from SciDAC Integrated Software Infrastructure Centers (ISIC) activities; discussions with members of the Algorithmic and Software Framework for Applied Partial Differential Equations ISIC about improved methods for matrix diagonalization

- Scientific accomplishments
  - Derivation and implementation of formulas for the first derivative of the CASPT2 energy in collaboration with the groups in Tromso Norway and Ferrara Italy
  - Reformulation of the CASPT2 equations in a way that lends itself more readily to differentiation and allows for more efficient parallelization.

- New software capabilities
  - Developed a technique for closed-shell systems that provides much higher accuracy that conventional methods and is much more scalable (even small systems involving half a dozen atoms can be run efficiently on 1000 processors!).

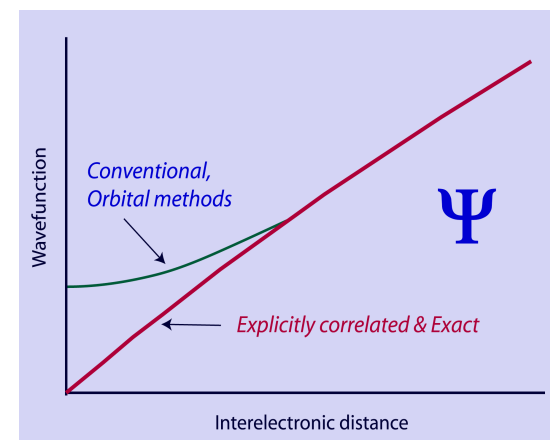# Accurate Properties for Open-Shell States of Large Molecules

Peter R. Taylor, University of Warwick

- Future plans
  - Couple recently developed closed shell technique to the CASPT2 method to treat open shells with plans to examine fitting methods that will extend this to molecules of perhaps hundreds of atoms.
  - Take advantage of the rather weak coupling, e.g. between metal atoms, to develop a factorization of the problem into a set of sub-problems; sub-problems will be small enough to be treated using conventional techniques; implement new schemes for the coupling between the sub-problems.

Next-Generation, Explicitly-Correlated Electronic Structure Methods

Wesley D. Allen and Henry F. Schaefer III

- Research approach
  - Development of "linear R12" methods
  - New computer code to evaluate the plethora of nonstandard two-electron integrals required by R12 theories by means of a sophisticated architecture effective for functions of arbitrarily high angular momentum.

- Scientific accomplishments
  - Several chemical applications exhibiting unparalleled convergence of predictions toward the complete basis set (CBS) limit, including studies to pinpoint the problematic barriers to linearity of H_2O and SiC_2, and the heats of formation of HNCO and NCO.

- New software capabilities
  - New integral-direct R12 package, incorporated into existing massively parallel quantum chemical suite to take full advantage of terascale computing facilities.

Conventional, Orbital methods

Ψ

Explicitly correlated & Exact

Wavefunction / Interelectronic distance

Superiority of explicitly correlated (R12) methods in the cusp regions of many-electron wavefunctions.

Next-Generation, Explicitly-Correlated Electronic Structure Methods

Wesley D. Allen and Henry F. Schaefer III

- Future plans
  - Development and implementation of explicitly-correlated perturbation and coupled-cluster theories for open-shell species, both within less complicated unrestricted (UHF) formalisms and more difficult spin-adapted (ROHF) approaches.
  - Work to solve certain technical deficiencies in the standard approximations for many-electron integrals in R12 theory and thereby to usher in the full promise of the methodology.
  - Conjoin lower-order, explicitly-correlated methods with high-order conventional correlation treatments via the focal-point scheme of Allen and co-workers to most efficiently reach the ab initio limit of molecular quantum mechanics
  - Work with the Head-Gordon and Piecuch groups to find better means of obtaining auxiliary high-order, conventional coupled-cluster predictions and thereby to more reliably infer exact correlation (FCI) limits.
  - Work with the Thompson group to develop improved methods for generating and representing large regions of potential energy hypersurfaces to address issues of chemical reaction dynamics with our next-generation electronic structure methods

Advanced methods for electronic structure: local coupled cluster theory

Martin Head-Gordon, LBNL

- Research approach
  - Develop powerful "local correlation" models that reduce scaling of coupled cluster calculations; develop the effective algorithms for their implementation.
  - Test and develop local CC methods which operate in a valence active space
  - Test the validity of using this valence space approximations in CC calculations, by comparing predicted molecular properties such as chemical bond-lengths and vibrational frequencies to CC theory without this approximation.

- Scientific accomplishments
  - Local correlation models have been combined with the valence space approximation to yield computationally efficient CC algorithms
  - Applied to large diradicaloid molecules, including models of a cleaved silicon surface, and a novel diborodiphosphino species recently isolated experimentally

Advanced methods for electronic structure: local coupled cluster theory

Martin Head-Gordon, LBNL

- New software capabilities
  - Efficient atomic-orbital driven algorithms for local CC models of this type have been implemented that reduce the computational cost of a local coupled cluster calculation to scale approximately cubically with the size of the molecule.
  - With a new computer large enough to do a conventional CC calculation on a molecule that is larger by a factor of x than one could do before, then this same computer would let one do a molecule x^2 larger with this local coupled cluster method!

Advanced methods for electronic structure: local coupled cluster theory

Martin Head-Gordon, LBNL

- Future plans
    - Generalization of the valence space approaches where the new local domain is an atom instead of an electron pair; only a linear number of degrees of freedom will be required, making a linear scaling algorithm possible; methods for both energies and analytical gradients will be developed.
    - Develop more accurate "fast methods" that still operate within the valence space approximation by adding additional ionic interpair excitations, while retaining only a quadratic number of degrees of freedom.
    - Combine simple valence local correlation model with Quantum Monte Carlo (QMC) methods; use the local CC wavefunction as a next generation choice of guiding function for fixed node diffusion QMC calculations, in collaboration with Prof. W.A. Lester (Berkeley).

Development Of New Scalable Multi-Reference Solutions For Electronic Structure, Dynamics and Non-Equilibrium Statistical Mechanics of Complex Reaction Processes

Mark S. Gordon, Iowa State University and Ames Laboratory (PI)

- Co-PIs:
  - Professor James W. Evans, Iowa State University and Ames Laboratory
  - Professor Klaus Ruedenberg, Iowa State University and Ames Laboratory
  - Dr. Michael W. Schmidt, Ames Laboratory
- Affiliated Researchers:
  - Professor Piotr Piecuch, Department of Chemistry, Michigan State University
  - Professor Brett M. Bode, Iowa State University and Ames Laboratory
  - Professor Ricky A. Kendall, Iowa State University and Ames Laboratory
  - Dr. Graham Fletcher, NASA Ames Research Center
  - Dr. Joseph Ivanic, National Cancer Institute

Development Of New Scalable Multi-Reference Solutions For Electronic Structure, Dynamics and Non-Equilibrium Statistical Mechanics of Complex Reaction Processes

Mark S. Gordon, Iowa State University and Ames Laboratory (PI)

- Research approach
  - Software developed in the electronic structure code GAMESS (General Atomic and Molecular Electronic Structure System); developed in such a way that it is easily implemented on any hardware and operating system.

- Scientific accomplishments
  - Highly scalable, distributed data and replicated data full CI (configuration interaction) codes; also available as the complete active space (CAS) component of CAS self-consistent field (SCF) methods.
  - Developed and implemented into GAMESS a more general multi-configurational (MC)SCF method that dramatically reduces the computational effort.
  - A very efficient second order CI (SOCI) capability has now been implemented in GAMESS.

Development Of New Scalable Multi-Reference Solutions For Electronic Structure, Dynamics and Non-Equilibrium Statistical Mechanics of Complex Reaction Processes

Mark S. Gordon, Iowa State University and Ames Laboratory (PI)

- – A suite of coupled cluster (CC) methods for the study of ground electronic states has now been implemented in GAMESS
- – A kinetic Monte-Carlo code was developed to describe the complex interplay between surface reaction processes and nanostructure formation during etching and oxidation of Si(100). Modeling was guided by *ab-initio* results for key energies

- New software capabilities
  - – All new capabilities distributed within GAMESS at no cost; currently has a registered user base of nearly 9,000.
  - – New GAMESS developments are often shared with others, especially the developers of NWChem at PNNL; benefiting both laboratories as well as the general user community.

- Future plans
  - – New approach (ORMAS) has been developed and will be implemented (with energy gradients); the active space can be subdivided into sets of smaller spaces, thereby greatly increasing the size of a system that can be studied.

Development Of New Scalable Multi-Reference Solutions For Electronic Structure, Dynamics and Non-Equilibrium Statistical Mechanics of Complex Reaction Processes

Mark S. Gordon, Iowa State University and Ames Laboratory (PI)

- higher order electron correlation methods will be developed for ORMAS, such as SOCI
- The CC codes in GAMESS will be broadened to include excited electronic states; open shell capabilities will be developed in subsequent years.
- Efficiency of the most sophisticated methods, like SOCI, will be optimized and made more scalable.
- Analytic gradients will be developed and implemented into GAMESS for several of the correlated methods.
- MCSCF Hessians will be developed and implemented.
- Codes will be developed that utilize kinetic Monte Carlo and other mesoscale modeling approaches

- Computational resource needs
  - The primary need is for significant amounts of time (on the order of 500,000 node hours/year) on the NERSC systems.

New Coupled-Cluster Methods for Molecular Potential Energy Surfaces

Piotr Piecuch, Department of Chemistry, Michigan State University (PI)

- Affiliated Researchers (SciDAC):
    - Professor Mark S. Gordon, Iowa State University and Ames Laboratory
    - Dr. Michael W. Schmidt, Associate Scientist, Ames Laboratory
- Interactions with Other SciDAC Participants:
    - Dr. Robert J. Harrison, Oak Ridge National Laboratory
    - Dr. David J. Dean, Oak Ridge National Laboratory
- Other collaborators:
    - Professor Stanislaw A. Kucharski, University of Silesia, Poland
    - Dr. Monika Musial, University of Silesia, Poland
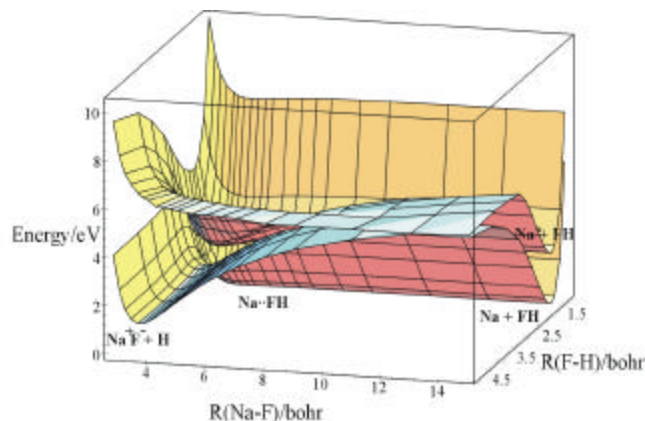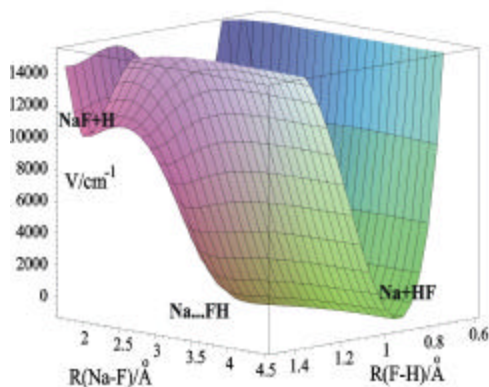
New Coupled-Cluster Methods for Molecular Potential Energy Surfaces

> Piotr Piecuch, Department of Chemistry, Michigan State University (PI)

- Research approach
  - develop "black-box" and yet very accurate coupled-cluster (CC) methods and computer codes that can provide an excellent description of bond breaking, reaction intermediates, molecular potential energy surfaces, and excited electronic states.

- Scientific accomplishments
  - New CC approaches: the *renormalized coupled-cluster methods*, the *active-space coupled-cluster methods*, and the *method of moments of coupled-cluster equations (MMCC)* capable of describing entire molecular potential energy surfaces and excited states at a fraction of the effort associated with the more traditional multi-reference configuration interaction (MRCI) calculations.
  - New methods applied to much larger systems and basis sets, and new chemical problems that could not be handled by the existing CC and MRCI approaches; demonstrated on systems consisting of 20-30 light atoms, clusters of ~10 transition metal atoms, and hundreds of basis functions.

New Coupled-Cluster Methods for Molecular Potential Energy Surfaces

Piotr Piecuch, Department of Chemistry, Michigan State University (PI)

- New software capabilities
  - Codes are fully vectorized and can access large memories (many GBs) available on the state-of-the-art computer platforms. Our CC codes are shared with the entire community by incorporating them in GAMESS.
  - Standard closed-shell CC approaches (LCCD, CCD, CCSD, CCSD[T], and CCSD(T)), and new and highly promising renormalized CCSD[T] and CCSD(T) methods for single bond breaking have been implemented.
  - The MMCC and renormalized CC methods have been extended to excited electronic states
  - The renormalized CC and MMCC methods have been extended to multiple bond breaking by developing the *quadratic MMCC, CI-corrected MMCC,* and *extended CC* methods.
  - A strong evidence has been provided that the exact many-electron wave functions can be represented by cluster expansions employing two-body operators.

New Coupled-Cluster Methods for Molecular Potential Energy Surfaces

Piotr Piecuch, Department of Chemistry, Michigan State University (PI)

- Future plans
    - Equation-of-motion CC (EOMCC), MMCC, and renormalized CC methods for excited electronic states will be developed.
    - The efficient codes for the new MMCC methods for multiple bond breaking will be developed.
    - Open-shell extensions of the CC/EOMCC and new MMCC, renormalized CC, and active-space CC methods will be developed.
    - Initial efforts will be made to parallelize the CC codes already in GAMESS

- Computational resource needs
    - In order to apply the developed codes to larger molecular problems relevant to combustion, photochemistry, and catalysis, there is a need for 200,000 node hours/year on the NERSC systems
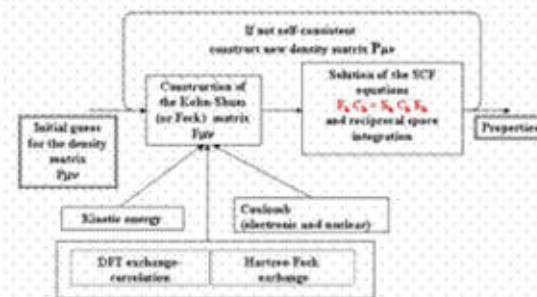
Linear Scaling Electronic Structure Methods with Periodic Boundary Conditions

Gustavo E. Scuseria, Rice University

- Research approach
  - Computational methods and tools are being adapted and expanded to deal with periodicity (*ie*, polymers, surfaces, and infinite solids) which will significantly enhance the current capabilities of the scientific community to model and study periodic systems.

General structure of the periodic Kohn-Sham DFT program.

- Scientific accomplishments
  - MP2 for periodic systems
  - Brillouin zone integration in metallic systems
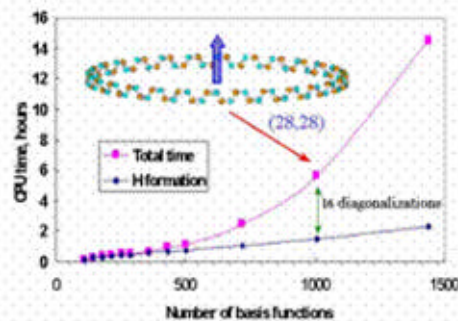 - Alternatives to the Hamiltonian diagonalization.

Computational scaling of our current implementation of the program

Linear Scaling Electronic Structure Methods with Periodic Boundary Conditions

Gustavo E. Scuseria, Rice University

- New software capabilities
  - an atomic-orbital formulation of second-order Møller–Plesset (MP2) theory for periodic systems has been developed.
    - The inherent spatial decay properties of the density matrix in the atomic orbital basis are exploited to reduce computational cost and scaling.
    - The multidimensional k-space integration is replaced by independent Fourier transforms of weighted density matrices.
    - The correlated amplitudes in the atomic orbital (AO) basis are obtained in closed-form, compatible with a semi-direct algorithm, thanks to the Laplace transform of the energy denominator.
    - The Laplace quadrature can be accurately carried out by using few integration points, 3 to 7 depending on the application.

Linear Scaling Electronic Structure Methods with Periodic Boundary Conditions

Gustavo E. Scuseria, Rice University

- An efficient algorithm for band connectivity (BC) resolution was developed.
  - The method uses only readily available band coefficients and the overlap matrix, and has a low computational cost.
  - The accuracy of the BC resolution is such that the method is practical for meshes of **k** points typically used in systems with small unit cells.
- Proposed a powerful approach to purification of the first-order density matrix based on minimizing the trace of a fourth-order polynomial, representing the deviation from idempotency.
  - Two variants: a robust and efficient steepest descent minimization, especially when the trial density matrix is far from idempotency and a quadratically convergent Newton–Raphson technique, if the trial matrix is nearly idempotent.

- Future plans
  - Implementations targeting terascale computers.

Relativistic Quantum Chemistry Software

Russell M. Pitzer (PI), Bruce E. Bursten, Isaiah Shavitt, Ohio State University

- Affiliated Researchers (SciDAC):
    - Professor Walter C. Ermler, University of Memphis
    - Professor Maria Marino, University of Memphis
- Other collaborators:
    - Professor Hans Lischka, University of Vienna
    - Dr. Ron Shepard, Argonne National Laboratory
    - Ohio Supercomputer Center, Software Repository

Relativistic Quantum Chemistry Software

Russell M. Pitzer (PI), Bruce E. Bursten, Isaiah Shavitt, Ohio State University

- Research approach
    - Software which includes relativistic effects is developed within the COLUMBUS suite of programs
- Scientific accomplishments
    - Parallelization, porting and testing of the COLUMBUS has been accomplished on some scientific platforms
    - The UO2 molecule (radical) has been studied with a present version of the Columbus programs; need for flexible wave function methods quite apparent.
- New software capabilities
    - New parallel version of COLUMBUS

Relativistic Quantum Chemistry Software

Russell M. Pitzer (PI), Bruce E. Bursten, Isaiah Shavitt, Ohio State University

- Future plans
  - Additional parallelization, porting and testing to other computer platforms continues
  - Scalability will be enhanced by converting current memory allocation methods to fortran 90, as well as updating a number of other features.
  - Other test cases are being developed
    - the interaction of $B_{10}H_{14}$ with I^- (known complex) and with Xe (unknown complex)
    - the intensities of lanthanide transitions in crystals, such as Er^{3+} doped into GaN.
- Computational resource needs
  - In order to study larger problems several hundred thousand node hours/year will be required on the CCS system.

Reliable Electronic Structure Calculations for Heavy Element Chemistry: *Relativistic Pseudopotentionals for Very-Large-Core Lanthanide and Actinide Systems*

Professor Walter C. Ermler, Professor Maria M. Marino, The University of Memphis

- Affiliated Researchers (SciDAC):
  - R. M. Pitzer, B. E. Bursten and I. Shavitt, Ohio State University.
- Other collaborators:
  - D. A. Dixon, W. A. de Jong, T. L. Windus, and M. Gutowski of the William R. Wiley Enviornmental Molecular Sciences Laboratory of PNNL
  - J. L. Tilson, Center for Computational Research (CCR), SUNY, Buffalo
  - A. F. Wagner, R. Shepard, ANL

Reliable Electronic Structure Calculations for Heavy Element Chemistry: *Relativistic Pseudopotentionals for Very-Large-Core Lanthanide and Actinide Systems*

Professor Walter C. Ermler, Professor Maria M. Marino, The University of Memphis

- Research approach
  - A relativistic pseudopotentional (RPP), that extends the usual two-space representation of atomic electrons (core and valence) to three spaces (core, outer core and valence) is under development within the COLUMBUS and NWChem suites of programs.

- Scientific accomplishments
  - New RECPs and RPPs for use in *ab initio* molecular electronic calculations have been developed

- New software capabilities
  - The use of RPPs in COLUMBUS and NWChem in conjunction with advanced computing platforms will permit the highly accurate *ab initio* treatment of systems possessing orders of magnitude more electrons than are tractable using current codes and platforms

Reliable Electronic Structure Calculations for Heavy Element Chemistry: *Relativistic Pseudopotentionals for Very-Large-Core Lanthanide and Actinide Systems*
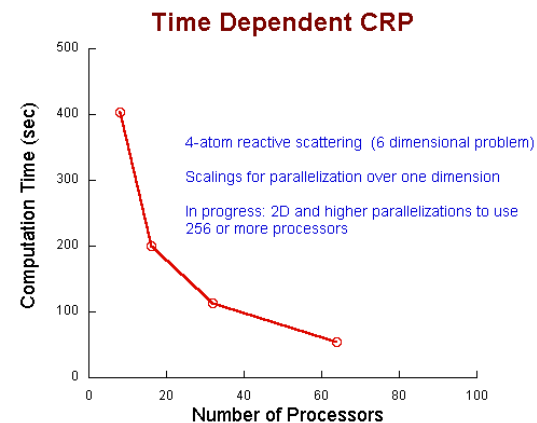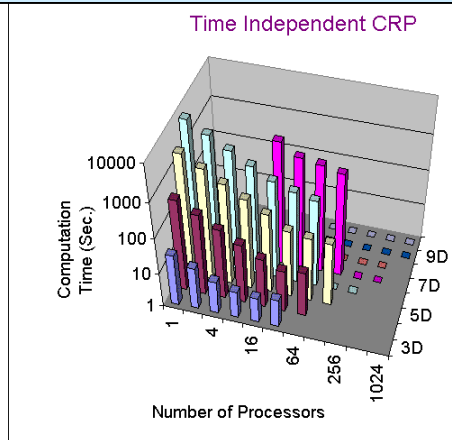
Professor Walter C. Ermler, Professor Maria M. Marino, The University of Memphis

- Future plans
    - Continue the computer implementation, formalism and calculation of RPPs for the individual elements, initially Am and Cl.
    - Continue generating the angular momentum projection operators to be associated with the RPPs.
    - Continue coding modules for molecular calculations utilizing the RPP
    - Upon completion of algorithm development and coding, implementation of the RPP formalism into the NWChem and Columbus suites will be carried out in collaboration with PNNL/EMSL and OSU/OSC, respectively.
    - large-scale SOCI benchmark calculations on $AmCl^{1+}$ will be carried out in collaboration with CCR.
    - Additionally, code optimization and parallelization, as well as the efficient two-, three- and four-center extensions of the RPP molecular codes will be carried out in collaboration with the SciDAC Centers.

Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamics
and
Theoretical Chemical Dynamics Studies for Elementary Combustion Reactions

Albert Wagner, ANL (PI) and Donald Thompson, OSU (PI)

- Co-PIs
  - Stephen Gray, ANL
  - Ron Shepard, ANL
  - Michael Minkoff, ANL
- ISIC co-PIs:
  - CCTTSS:
    - Lois McInnes, ANL
    - Dave Bernholdt, Oak Ridge National Laboratory
  - TOPS:
    - Michael Minkoff, ANL
    - Barry Smith, ANL

Time Independent CRP

Legend: 3D, 4D, 5D, 6D

Computation Time (Sec.) vs Number of Processors

Time Dependent CRP

Computation Time (sec) vs Number of Processors

4-atom reactive scattering (6 dimensional problem)

Scalings for parallelization over one dimension

In progress: 2D and higher parallelizations to use 256 or more processors

Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamic & Theoretical Chemical Dynamics Studies for Elementary Combustion Reactions

Albert Wagner, ANL (PI) and Donald Thompson, OSU (PI)

- Research approach
  - Formalisms for both time-independent and time-dependent Cumulative Reaction Probability (CRP) exact rate constants are being developed.
- Scientific accomplishments
  - A parallelized time independent CRP code has been developed on top of the PETSc library; code testing on model problems with analytic CRP solution is underway.
  - A parallel, four-atom, 6 degrees of freedom (DOF), time-dependent CRP code has been developed; parallelization has been accomplished over several DOF using the message passing interface OpenMP which allows both shared memory for all the processors within a node but message passing between processors on different nodes.
  - Convenient ways to produce and use PESs that reduce the number of electronic structure calculations needed for accurate kinetics/dynamics are being developed.

Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamic & Theoretical Chemical Dynamics Studies for Elementary Combustion Reactions

Albert Wagner, ANL (PI) and Donald Thompson, OSU (PI)

- – Preconditioner approaches for the numerics of kinetics/dynamics applications but with implications for electronic structure applications are being developed
- – Higher order Interpolative Moving Least Squares (IMLS) PES fitting methods are being explored.
- – Conversion of POTLIB 2001 (a program library of PESs with a common, published user interface for every library entry) to common component architecture (CCA) compliance is underway.
- – A multigrid-like preconditioner for large-scale iterative eigensolvers where matrix-vector products dominate the solution is being developed called the Subspace Projected Approximate Matrix (SPAM) method.
- New software capabilities
  - – The time independent CRP code is scalable over a hundred or more processors with time to solutions at NERSC measured at about ten minutes per eigenvalue for a 7 DOF problem.

Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamic & Theoretical Chemical Dynamics Studies for Elementary Combustion Reactions

Albert Wagner, ANL (PI) and Donald Thompson, OSU (PI)

– Tests have been performed using the time dependent CRP code on up to 256 processors (16 processors per 16 nodes); code tuning is in progress. The OpenMP strategy of intra-node shared memory parallelization and inter-node message passing parallelization maps well onto CRP problems with more atoms and more DOF.

– Fortran95 "black box" code for symmetric, Hermitian, or real generalized symmetric eigenvalue problems have been developed within SPAM

- Future plans

  – Global preconditioners including the Subspace Projected Approximated Matrix approach and optimal block orthogonal preconditioning will be examined

  – After code tuning and tests on selected applications, the scalability of the code with processor/node combinations and with higher DOF will be explored.

  – SPAM parallel extensions are being developed based on distributed-memory message passing (e.g. MPI), on the global array library, and on the PETSc environment.